Proposal

Title – ChemSIM: Visualizing Chemical Equilibrium through a Java-Based Program

Programs of Study – Chemistry and Electrical Engineering

Presentation Type – Print Poster

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Category – Theoretical Proposal

Abstract – ChemSIM is a Java-based program designed to aid general chemistry students as well as physical chemistry students in the visualization of the processes involved with establishing chemical equilibrium. Chemical equilibrium, which is considered to be the time point in a chemical process at which the forward and reverse rates of a particular reaction are equal, is affected by the initial concentrations of the chemical species as well as the pressure and temperature conditions surrounding the reaction. The program will be interfaced such that the user can manipulate certain parameters like the initial velocities of the model species, the masses of the species, the concentrations of the different species, and the pressure and temperature conditions in order to visualize how these physical constraints affect the establishment of chemical equilibrium. In contrast to the traditional method of teaching collision theory, ChemSIM utilizes a method that is independent of the impact parameter, b, for modeling hard-sphere collisions. The method employed by the program utilizes the initial velocities of two atoms and the masses to calculate the total momentum of the system, which subsequently allows for a calculation of the final velocities of the atoms following the collision.

Additionally, ChemSIM's method of calculating the velocities of the atoms allows for a simple method of assessing the energy of the system, thereby allowing the user to visualize, via a color change, if two model atoms collided with sufficient energy for the particular reaction with activation energy, E_a, to occur. With the foundation in place, ChemSIM can be expanded to describe more complex molecular systems, as in organic and biochemistry, where orientation of the molecules during collision is an important constraint affecting whether or not a reaction occurs.